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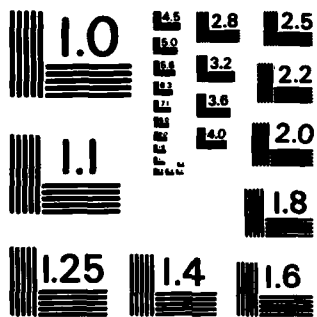
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| 19. ABSTRACT (Continue on reverse if necessary and identify by block number) Fast algorithms for solving numerical problems involving large sparse matrix computations are investigated. Applications of this work to the areas of structural analysis, constrained optimization and large scale least squares adjustment methods are developed. One of the more important accomplishments is the design and testing on the Denelcor HEP multiprocessor of a parallel algorithm for computing a banded basis matrix for the null space. This algorithm may lead to a new efficient sparse matrix implementation of the force method for the finite element analysis of large-scale structures. | | | | | | | | | | | | |
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MATTHEW J. KERTNER

I. RESEARCH OBJECTIVES, Technical Information Division

The research problems studied during the first year of this grant were concerned with sparse matrix technology in structural analysis, least squares geodetic adjustments and related problems in science and engineering. The objectives of this research were to develop fast numerical algorithms for the efficient solution to large-scale systems of linear equations $Ax = b$ and least squares problems $\min_x ||b - Ax||_2$, where A is large and sparse and often has a special structured form.

One particular project to be undertaken involved the development and testing of serial and parallel algorithms for null space computations associated with the efficient implementation of the force method for the stress analysis of large-scale structures. A second major project involved the development of direct-iterative methods for large sparse least squares and constrained minimization problems associated with structural analysis and with the adjustment of large amounts of geodetic data. The major results obtained thus far on these projects are outlined in the next section.

II. SUMMARY OF MAJOR RESULTS

The most important research accomplishments by the principal investigator and co-workers are described below. These results have been obtained on five specific problems in computational mathematics and applications.

1. Sparse Orthogonal Schemes for Structural Optimization using the Force Method.

Historically there are two principal methods of matrix structural analysis, the displacement (or stiffness) method and the force (or flexibility) method. In recent times the force method has been used relatively little because the displacement method has been deemed easier to implement on digital computers, especially for large sparse systems. The force method has theoretical advantages, however, for multiple redesign problems or nonlinear elastic analysis because it

allows the solution of modified problems without restarting the computation from the beginning. In this work an implementation of the force method is given which is numerically stable and preserves sparsity. Although it is motivated by earlier elimination schemes, in this approach each of the two main phases of the force method is carried out using orthogonal factorization techniques recently developed for linear least squares problems by George, Golub, Heath and Plemmons.

2. An Algorithm to Compute a Sparse Basis of the Null Space.

Let A be a real $m \times n$ matrix with full row rank m . In many algorithms in engineering and science, such as the force method in structural analysis, the dual variable method for the Navier-Stokes equations or more generally null space methods in quadratic programming, it is necessary to compute a basis matrix B for the null space of A . Here B is $n \times r$, $r = n - m$, of rank r , with $AB = 0$. In many instances A is large and sparse and often banded. The purpose of this work was to describe and test a variation of a method originally suggested in Germany and called the turnback algorithm for computing a banded basis matrix B . Two implementations of the algorithm were developed, one using Gaussian elimination and the other using orthogonal factorization by Givens rotations. The FORTRAN software was executed on an IBM 3081 mainframe computer with and FPS-164 attached array processor at the Triangle Universities Computing Center near Raleigh, N. C. Test results on a variety of structural analysis problems including two- and three-dimensional frames, plane stress, plate bending and mixed finite element problems have been made. These results indicate that both implementations of the algorithm yielded a well-conditioned, banded, basis matrix B when A is well conditioned, but that the orthogonal scheme yielded a better conditioned B for large, ill-conditioned problems.

3. A Direct-Iterative Method for Large-scale Least Squares Problems.

IN 1975 Chen and Gentleman suggested a 3-block SOR method for solving least squares problems, based on a partitioning scheme for the observation matrix A into:

$$A = \begin{bmatrix} A_1 \\ A_2 \end{bmatrix}$$

where A_1 is square and nonsingular. In many cases A_1 is obvious from the nature of the problem. This combined direct-iterative method was discussed further and applied to angle adjustment problems in geodesy, where A_1 is easily formed

and is large and sparse, by Plemmons in 1979 for the Army Research Office. Recently, Niethammer, de Pillis and Varga have rekindled interest in this method by correcting and extending the SOR convergence interval. The purpose of our work here was to provide an alternate formulation of the problem leading to a 2-block SOR method. For this formulation it was shown that the resulting direct-iterative method always converges for sufficiently small SOR parameter, in contrast to the 3-block formulation. Formulas for the optimum SOR parameter and the resulting asymptotic convergence factor were derived. Furthermore, it was shown that this 2-cyclic block SOR method always gives better convergence results than the 3-cyclic case for the same amount of work per iteration.

4. Applications of a Block SOR Method to a Class of Constrained Minimization Problems.

In this work it is shown how a block successive overrelaxation direct-iterative method can be applied to the solution of a class of linear equality-constrained quadratic programming problems. The scheme is similar in nature to those studied recently by de Pillis, Niethammer and Varga and by Markham, Neumann and Plemmons for solving large sparse least squares problems. It is based upon a partitioning strategy of the fundamental matrix into a block consistently ordered 2-cyclic form where the nonzero eigenvalues of the Jacobi matrix are all pure imaginary. Applications of the method to structural optimization problems have been developed in this research.

5. Computing a Banded Basis of the Null Space on the Denelcor HEP Multiprocessor.

The banded null space basis problem is the following: given an $m \times n$ banded matrix A of rank $m < n$, find a banded $n \times (n - m)$ matrix B whose columns span the null space of A , i.e., find a banded B of rank $n - m$ with $AB = 0$. This problem arises in the design of practical algorithms for large-scale numerical optimization problems in engineering and science, such as the force method in structural analysis, the dual variable method for solving the Navier-Stokes equations in fluid mechanics or more general problems in linearly and nonlinearly constrained minimization.

The purpose of this work is the design and testing of a parallel version of a highly effective but intensive turnback algorithm for computing a banded basis matrix B . The turnback algorithm is shown to exhibit a moderate amount of modular parallelism. FORTRAN codes for both the serial and parallel versions of the algorithm have been implemented on the Denelcor HEP

computer at the Argonne National Laboratory, and MIMD multiprocessing machine. Performance results using some practical data from structural analysis problems indicate that our parallel implementation executes significantly faster than the serial implementation.

III. RESEARCH IN PROGRESS

Two research projects in support of this grant are currently underway and are briefly described below. A more complete description of this current work will be given in next year's annual scientific report.

1. Accurate Finite Element Calculations for Large-Scale Structures.

Here a new approach to calculating the vector f of internal forces and the associated stresses, given a finite element model of a structure and an external load vector p , is being undertaken. This approach is based upon solving the fundamental problem of linear elastic analysis

$$\min_f f^T F f \quad \text{subject to } E f = p$$

where F denotes the element flexibility matrix and E the equilibrium matrix, as a linearly constrained least squares problem. This least squares problem is then solved by a weighted least squares scheme using an iterative improvement scheme developed recently by C. Van Loan. Numerical comparisons are currently being made with the natural factor formulation of this problem in terms of accuracy and numerical efficiency. This work is joint with C. Van Loan in the Computer Science Department at Cornell University.

2. A Parallel Version of the Golub/Plemmons Algorithm for the Orthogonal Factorization of Least Squares Observation Matrices in Block Angular Form.

The Golub/Plemmons block orthogonal factorization algorithm was designed for the stable least squares adjustment of large amounts of geodetic data which is assembled so that the observation matrix has a bordered block diagonal form. The algorithm also applied to more general substructuring or domain decomposition methods. In this work it is being investigated how a parallel version of the algorithm can be applied not only to the factorization scheme but also to the back substitution phase of the least squares method. The algorithm is being programmed for testing on the Denelcor HEP multiprocessing computer at the Argonne National Lab. This is joint work with A. Sameh in the Computer Science Department at the University of Illinois.

IV. TECHNICAL PUBLICATIONS.

1. "Minimum Norm Solutions to Linear Elastic Analysis Problems", Inter. J. Numer. Meth. in Engineering, 20(1984), 983-998 (with I. Kaneko).
2. "Sparse Orthogonal Schemes for Structural Optimization Using the Force Method", SIAM J. Sci. and Statistical Computing, 5(1984), 514-532 (with M. Heath and R. Ward).
3. "An Algorithm to Compute a Sparse Basis of the Null Space", to appear in Numerische Mathematik (with M. Berry, M. Heath, I. Kaneko, M. Lawo and R. Ward).
4. "Convergence of a Direct-Iterative Method for Large-Scale Least Squares Problems", to appear in Linear Algebra and Its Applications (with T. Markham and M. Neumann).
5. "Computing a Banded Basis of the Null Space on the Denelcor HEP Multiprocessor", Proc. of the SIAM/AMS Conference on Linear Algebra in Systems Theory, to appear in the AMS series on Contemporary Mathematics (with M. Berry).
6. "Application of a Block SOR Method to a Class of Constrained Minimization Problems", submitted to Mathematics of Computation.
7. "Accurate Finite Element Calculations for Large-Scale Structures", in preparation, may be submitted to Computers and Structures (with C. Van Loan).
8. "Solving Structured Least Squares Problems by Block Orthogonal Factorization on the Denelcor HEP Multiprocessor", in preparation, may be submitted to Linear Algebra and Its Applications (with A Sameh).

V. PROFESSIONAL PERSONNEL ASSOCIATED WITH THE RESEARCH EFFORT

R. J. Plemmons - Principal Investigator

M. W. Berry - Graduate Research Assistant

VI. INVITED PRESENTATIONS AND RELATED ACTIVITIES.

The following invited lectures were given by the principal investigator at research conferences and meetings.

1. "Convergence of Gauss-Seidel Iterations on Some Large Sparse Problems," Conference on Linear Algebra and Applications, Vitoria, Spain, October, 1983.

2. "Large-Scale Least Squares Problems", Conference on the Impact of Large-Scale Computing on Air Force Research and Development, Albuquerque, New Mexico, April, 1984.
3. "Block Direct-Iterative and Null Space Methods for Least Squares and Constrained Minimization Problems", Gatlinburg IX Conference on Numerical Linear Algebra, Waterloo, Canada, July, 1984.

The principal investigator participated in the following workshop activities.

1. Workshop on Supercomputers and Least Squares, organized by J. R. Rice and supported by the ONR and the ARO, Purdue, Indiana, November, 1983.
2. NSF Workshop on Supercomputer Access, Boulder, Colorado, February, 1984.
3. Argonne National Laboratory Workshop on the Denelcor HEP Multiprocessor, Argonne, Illinois, June, 1984.

In addition, the principal investigator organized a minisymposium, Parallel and Vector Algorithms for Matrix Computations, at the SIAM Fall Meeting, Norfolk, Virginia, November, 1983, as Chairman of the SIAM Activity Group on Linear Algebra.

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